

# Itinerant ferrimagnetism on $AB_2$ Hubbard chains: Charge and spin quantum fluctuations

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The ground state (GS) properties of the ferrimagnetic quasi-one-dimensional  $AB_2$  Hubbard model are calculated taking the effects of charge and spin quantum fluctuations on equal footing. Using a functional integral approach, combined with a perturbative expansion in the strong-coupling regime, we derive the Lagrangian density associated with the charge (Grassmann fields) and spin [ $SU(2)$  gauge fields] degrees of freedom. In the strong-coupling regime ( $U \gg t$ , where  $U$  is Coulomb repulsion and  $t$  is the first-neighbor hopping amplitude), we obtain a perturbative low-energy theory suitable to describe the ferrimagnetic phase at half filling and in the hole-doped regime. At half filling, by applying a perturbative expansion in powers of  $1/S$  (spin-wave analysis), we find that the GS energy, sublattice magnetizations, and Lieb total spin per unit cell of the quantum Heisenberg model are in good agreement with previous results. In the challenging doped regime, we obtain the corresponding  $t$ - $J$  ( $= 4t^2/U$ ) Hamiltonian. Notably, our analytical results for the GS energy and total spin per unit cell as a function of hole doping away from half filling are in very good agreement with recent numerical estimates, particularly in the regime where the Nagaoka phenomenon is not manifested. In fact, in this regime, charge and spin quantum fluctuations are practically decoupled, as numerically indicated by the formation of charge-density waves in anti-phase with the modulation of the ferrimagnetic structure.

## I. INTRODUCTION

Much attention has been given to quantum phase transitions<sup>1–3</sup>, which are phenomena characterized by the change of the nature of the ground state (GS) driven by a non-thermal parameter: pressure, magnetic field, doping, Coulomb repulsion, or competitive interactions. In this context, the study of quasi-one-dimensional (quasi-1D) compounds with ferrimagnetic properties<sup>4,5</sup> has attracted considerable theoretical and experimental interest because of their unique physical properties and very rich phase diagrams. In particular, the GS of quasi-1D quantum ferrimagnets with  $AB_2$  or  $ABB'$  unit cell topologies described by the Heisenberg or Hubbard models<sup>6</sup> exhibit unsaturated spontaneous magnetization, ferromagnetic and antiferromagnetic spin-wave modes, effect of quantum fluctuations, and field-dependent magnetization plateaus.

Of special interest is the topological origin of the GS long-range order related to the unit cell structure of the lattice<sup>6–13</sup>. These studies have been motivated and supported by exact solutions and rigorous results<sup>14–19</sup>; in particular, at half filling, the total spin per unit cell obeys Lieb-Mattis<sup>14</sup> (Heisenberg model) or Lieb's theorem<sup>16</sup> (Hubbard model). On the other hand, it has been verified that the ferrimagnetic GS of spin-1/2 Heisenberg or Hubbard /  $t$ - $J$   $AB_2$  chains, under frustration<sup>20–24</sup> or doping<sup>8,12,25,26</sup>, is strongly affected by enhanced quantum fluctuations that might cause its destruction and the occurrence of new exotic phases: spiral, Nagaoka ( $U \rightarrow \infty$ ) and resonating-valence-bond states, phase separation, and Luttinger-liquid behavior. In addition, investigations of transport properties in  $AB_2$  chains, and related structures, have unveiled very interesting features<sup>27</sup>.

On the experimental side, studies<sup>28–30</sup> of the mag-

netic properties of homometallic phosphate compounds of the family  $A_3Cu_3(PO_4)_4$ ,  $A = Ca, Sr$ , and  $Pb$  suggest that in these materials the line of trimers formed by spin-1/2  $Cu^{+2}$  ions antiferromagnetically coupled do exhibit ferrimagnetism of topological origin. On the other hand, bimetallic compounds, such as  $CuMn(S_2C_2O_2)_2 \cdot 7.5H_2O$ <sup>31</sup>, can be modeled<sup>31–33</sup> by alternate spin-1/2 - spin-5/2 chains and support interesting field-induced quantum critical points and Luttinger-liquid phase. In addition, frustrated diamond ( $AB_2$  topology) chains can properly model the compound azurite,  $Cu_3(CO_3)_2(OH)_2$ , in which case the occurrence of the 1/3 (in comparison with the saturation value) magnetization plateau is verified at high fields<sup>34</sup> in agreement with topological arguments<sup>35</sup> akin to those invoked in the quantum Hall effect. The spin-1/2 trimer chain compound  $Cu_3(P_2O_6OH)_2$ , with antiferromagnetic interactions only, also display the 1/3 magnetization plateau<sup>36</sup>. Interestingly, it has been established that in azurite the magnetization plateau is a dimer-monomer state<sup>37</sup>, i.e., the chain is formed by pairs of  $S = 1/2$  monomers and and  $S = 0$  dimers. These dimer-monomer states have been found previously in the context of modeling frustrated  $AB_2$  chains<sup>38–40</sup>, and confirmed through a modeling using quantum rotors<sup>41</sup>.

In this work, we shall employ an analytical approach suitable to describe the strongly coupled Hubbard model on doped  $AB_2$  chains, which were the object of recent numerical studies through DMRG techniques<sup>26</sup>. Our functional integral approach, combined with a perturbative expansion in the strong-coupling regime, was originally proposed to study the doped Hubbard chain<sup>42</sup>, and latter adapted to describe various doped-induced phase transitions in the  $U = \infty$   $AB_2$  Hubbard chain<sup>43</sup>. Very recently, this approach was used to describe the doped strongly

coupled Hubbard model on the honeycomb lattice<sup>44</sup>, whose results are very rewarding, particularly those for the GS energy and magnetization in the doped regime, which compare very well with Grassmann tensor product numerical studies<sup>45</sup>. The effect of quantum fluctuations is most effectively appreciated in a very recent study of the Kagome lattice compound  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ <sup>46</sup> under electron doping, in which case, and against theoretical expectations<sup>47</sup>, the quantum spin-liquid phase is robust up to the observed doped-induced systematic suppression of magnetic behavior.

The paper is organized as follows: in Sec. II we review the functional integral representation of the Hubbard Hamiltonian in terms of Grassmann fields (charge degrees of freedom) and spin  $SU(2)$  gauge fields (spin degrees of freedom). In Sec. III we diagonalize the Hamiltonian associated with the charge degree of freedom and obtain a perturbative low-energy theory suitable to describe the ferrimagnetic phase at half filling and in the hole-doped regimes. The derivation of this perturbative expansion is shortly presented in Appendix. In Sec. IV, we show that the resultant Hamiltonian at half filling and large- $U$ , maps onto the spin-1/2 quantum Heisenberg model. In this regime, a perturbative series expansions in powers of  $1/S$  of the low-lying excitations of the referred Hamiltonian is presented, which allows us to calculate the GS energy and sublattice magnetizations, in very good agreement with previous estimates. In Sec. V, we derive the low-energy effective  $t$ - $J$  Hamiltonian, which accounts for both charge and spin quantum fluctuations. Our analytical results for the GS energy and total spin per unit cell as a function of hole doping away from half filling are in very good agreement with the recent numerical calculations, particularly in the regime where the Nagaoka phenomenon is not manifested. Lastly, in Sec. VI, we present a summary and concluding remarks concerning the reported results.

## II. FUNCTIONAL-INTEGRAL REPRESENTATION

The Hamiltonian of the one-band Hubbard model on chains with  $AB_2$  unit cell topology is given by<sup>8,9,11</sup>:

$$\mathcal{H} = - \sum_{\langle i\alpha, j\beta \rangle \sigma} \{t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} + \text{H.c.}\} + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow}, \quad (1)$$

where  $i = 1, \dots, N_c (= N/3)$  is the specific position of the unit cell,  $N_c$  ( $N$ ) is the number of cells (sites),  $\alpha, \beta = A, B_1, B_2$  denote the type of site within the unit cell,  $\hat{c}_{i\alpha\sigma}^\dagger$  ( $\hat{c}_{i\alpha\sigma}$ ) is the creation (annihilation) operator of electrons with spin  $\sigma$  ( $=\uparrow, \downarrow$ ) at site  $\alpha$  of cell  $i$ , and  $\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma}$  is the occupancy number operator. The first term in Eq. (1) describes electron hopping, with energy  $t_{ij}^{\alpha\beta} \equiv t$ , allowed only between nearest neighbors  $A$ - $B_1$  and  $A$ - $B_2$  linked sites of sublattices  $A$  and  $B$  (bipartite lattice), and the second one is the on-site Coulombian repulsive

interaction  $U > 0$ , which contributes only in the case of double occupancy of the site  $i\alpha$ .

At this point, it is instructive to digress on some fundamental aspects of the formalism used in our work<sup>42-44</sup>. With regard to the large- $U$  doped, Hubbard chain<sup>42</sup>,  $U = \infty$   $AB_2$  Hubbard chain<sup>43</sup> and the Hubbard model on the honeycomb lattice<sup>44</sup>, it has been shown that the particle density product in Eq. (1) can be treated through the use of a decomposition procedure, which consist in expressing  $\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow}$  in terms of charge and spin operators:

$$\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} = \frac{1}{2}\hat{\rho}_{i\alpha} - 2\left(\hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha}\right)^2, \quad (2)$$

where  $\hat{\mathbf{S}}_{i\alpha} = 1/2 \sum_{\sigma\sigma'} \hat{c}_{i\alpha\sigma'}^\dagger \boldsymbol{\sigma}_{\sigma'\sigma} \hat{c}_{i\alpha\sigma}$  and  $\hat{\rho}_{i\alpha} = \hat{n}_{i\alpha\uparrow} + \hat{n}_{i\alpha\downarrow}$ , are the spin-1/2 and charge-density operators, respectively,  $\boldsymbol{\sigma}_{\sigma'\sigma}$  denotes the Pauli matrix elements ( $\hbar \equiv 1$ ), and  $\mathbf{n}_{i\alpha}$  is a unit vector field along the spin quantization axis of an electron at site  $i\alpha$ . The identity in Eq. (2) will prove very useful in the context of the large- $U$  Hubbard model, since in this case, the on-site Coulomb repulsion ( $U$ ) between the electrons is very large as compared with the electron hopping energy  $t$ , making double occupancy energetically unfavorable, i.e., electrons become strongly correlated to avoid double occupancy.

We start by using the Trotter-Suzuki formula<sup>48</sup>, which allows us to write the partition function,  $\mathcal{Z} = \text{Tr}[\exp(-\beta\mathcal{H})]$ , at a temperature  $k_B T \equiv 1/\beta$ , as  $\mathcal{Z} = \text{Tr}\{\hat{T} \prod_{r=0}^{M-1} \exp[-\delta\tau \mathcal{H}(\tau_r)]\}$ , where  $\hat{T}$  denotes the time-ordering operator,  $\tau \in [0, \beta]$  is the imaginary-time formally sliced into  $M$  finite discrete intervals  $[\tau_r, \tau_{r+1})$  of equal size  $\delta\tau$ , where  $r = 0, 1, \dots, M-1$ ,  $\tau_0 = 0$ ,  $\tau_M = \beta$  and  $\beta = M\delta\tau$ , under the limits  $M \rightarrow \infty$  and  $\delta\tau \rightarrow 0$ . We shall now introduce, between each time interval, an over-complete basis of fermionic coherent states,  $1 = \int \prod_{i\alpha\sigma} d\hat{c}_{i\alpha\sigma}^\dagger d\hat{c}_{i\alpha\sigma} \exp(-\hat{c}_{i\alpha\sigma}^\dagger c_{i\alpha\sigma}) |c_{i\alpha\sigma}\rangle \langle c_{i\alpha\sigma}|$ , where  $\{c_{i\alpha\sigma}^\dagger, c_{i\alpha\sigma}\}$  denotes a set of Grassmann fields satisfying anti-periodic boundary conditions in the imaginary-time domain:  $c_{i\alpha\sigma}^\dagger(0) = -c_{i\alpha\sigma}^\dagger(\beta)$  and  $c_{i\alpha\sigma}(0) = -c_{i\alpha\sigma}(\beta)$ , while the unit vector field (see below) satisfies periodic ones:  $\mathbf{n}_{i\alpha}(0) = \mathbf{n}_{i\alpha}(\beta)$ . Thereby, the partition function takes the form:

$$\mathcal{Z} = \int \prod_{i\alpha} \mathcal{D}^2 \mathbf{n}_{i\alpha} \prod_{i\alpha\sigma} \mathcal{D} c_{i\alpha\sigma}^\dagger \mathcal{D} c_{i\alpha\sigma} \exp[-\int_0^\beta \mathcal{L}(\tau) d\tau], \quad (3)$$

where the measures are defined by

$$\mathcal{D}^2 \mathbf{n}_{i\alpha} \equiv \lim_{M \rightarrow \infty} \prod_r d^2 \mathbf{n}_{i\alpha}(\tau_r) W[\mathbf{n}_{i\alpha}(\tau_r)], \quad (4)$$

and

$$\mathcal{D} c_{i\alpha\sigma}^\dagger \mathcal{D} c_{i\alpha\sigma} \equiv \lim_{M \rightarrow \infty} \prod_r d\hat{c}_{i\alpha\sigma}^\dagger(\tau_r) d\hat{c}_{i\alpha\sigma}(\tau_r), \quad (5)$$

the normalized weight function:  $\int \prod_{i\alpha} d^2 \mathbf{n}_{i\alpha} W(\mathbf{n}_{i\alpha}) = 1$ , is given by  $W(\mathbf{n}_{i\alpha}) = \sqrt{\frac{\varphi}{\pi}} \exp\{-\varphi[\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} -$

$\frac{p_{i\alpha}}{2}\rho_{i\alpha}(2-\rho_{i\alpha})^2\}$  and  $\varphi \rightarrow \infty$  (delta-like limit). This representation is made possible by noticing the relation:  $(\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 = \frac{\rho_{i\alpha}(2-\rho_{i\alpha})}{4}$ , where the expectation value of the local charge-density operator is  $\rho_{i\alpha} = \langle \hat{\rho}_{i\alpha} \rangle = 0, 1$ , or 2, while  $\langle (\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 \rangle = (\pm 1/2)^2 = 1/4$ . Therefore, we can formally write that  $\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} = p_{i\alpha} \frac{\rho_{i\alpha}(2-\rho_{i\alpha})}{2}$ , which vanishes for double occupancy or vacancy, and the staggered factor obey  $p_{i\alpha} = +1$  ( $-1$ ) for sites  $\alpha = B_1, B_2$  ( $A$ ), according to the long-range ferrimagnetic GS predicted by Lieb's theorem<sup>16</sup> for the  $AB_2$  Hubbard chains at half filling. In this way, one is able to linearize the term  $(\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2$ . Therefore, the Lagrangian density  $\mathcal{L}(\tau)$  thus reads:

$$\begin{aligned} \mathcal{L}(\tau) = & \sum_{i\alpha\sigma} c_{i\alpha\sigma}^\dagger \partial_\tau c_{i\alpha\sigma} - \sum_{ij\alpha\beta\sigma} (t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + \text{H.c.}) \\ & + U \sum_{i\alpha} [\frac{\rho_{i\alpha}}{2} - p_{i\alpha}(\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha})]. \end{aligned} \quad (6)$$

Now, by considering the symmetry exhibited by the ferrimagnetic order, let us define the  $SU(2)/U(1)$  unitary rotation matrix,

$$U_{i\alpha} = \begin{bmatrix} \cos\left(\frac{\theta_{i\alpha}}{2}\right) & -\sin\left(\frac{\theta_{i\alpha}}{2}\right)e^{-i\phi_{i\alpha}} \\ \sin\left(\frac{\theta_{i\alpha}}{2}\right)e^{i\phi_{i\alpha}} & \cos\left(\frac{\theta_{i\alpha}}{2}\right) \end{bmatrix}, \quad (7)$$

where  $\theta_{i\alpha}$  is the polar angle between the  $z$ -axis and the unit local vector  $\mathbf{n}_{i\alpha}$ , and  $\phi_{i\alpha} \in [0, 2\pi)$  is an arbitrary azimuth angle due to the  $U(1)$  gauge freedom of choice for  $U_{i\alpha}$ , in which case the following relation obtains:  $U_{i\alpha}^\dagger(\boldsymbol{\sigma} \cdot \mathbf{n}_{i\alpha})U_{i\alpha} = \sigma^z$ , which explicitly manifest the rotationally broken symmetry along the  $z$ -axis. These definitions, along with the choice of  $p_{i\alpha}$  above, allow us to identify the ferrimagnetic ordering with the set  $\{\theta_{iA} = \theta_{iB_1} = \theta_{iB_2} = 0\}$  for all  $i$ . Moreover, a new set of Grassmann fields,  $\{a_{i\alpha\sigma}^\dagger, a_{i\alpha\sigma}\}$  can be obtained, according to the transformation:

$$a_{i\alpha\sigma} = \sum_{\sigma'} (U_{i\alpha})_{\sigma\sigma'}^\dagger c_{i\alpha\sigma'}, \quad (8)$$

whose associated spins point along the global  $z$ -axis. Substituting Eqs. (7) and (8) into the Lagrangian, Eq. (6), along with  $\mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} = S_{i\alpha}^z$  and  $\rho_{i\alpha}$  expressed in terms of  $\{a_{i\alpha\sigma}^\dagger, a_{i\alpha\sigma}\}$ , we find

$$\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \mathcal{L}_n(\tau), \quad (9)$$

where

$$\begin{aligned} \mathcal{L}_0(\tau) = & \sum_{i\alpha\sigma} a_{i\alpha\sigma}^\dagger \partial_\tau a_{i\alpha\sigma} - \sum_{ij\alpha\beta\sigma} (t_{ij}^{\alpha\beta} a_{i\alpha\sigma}^\dagger a_{j\beta\sigma} + \text{H.c.}) \\ & + \frac{U}{2} \sum_{i\alpha} (1 - p_{i\alpha}\sigma) a_{i\alpha\sigma}^\dagger a_{i\alpha\sigma}, \end{aligned} \quad (10)$$

and

$$\begin{aligned} \mathcal{L}_n(\tau) = & \sum_{i\alpha\sigma\sigma'} a_{i\alpha\sigma'}^\dagger (U_{i\alpha}^\dagger \partial_\tau U_{i\alpha})_{\sigma'\sigma} a_{i\alpha\sigma} \\ & - \sum_{i\alpha j\beta\sigma\sigma'} t_{ij}^{\alpha\beta} [a_{i\alpha\sigma'}^\dagger (U_{i\alpha}^\dagger U_{j\beta} - 1)_{\sigma'\sigma} a_{j\beta\sigma} + \text{H.c.}]. \end{aligned} \quad (11)$$

It is worth mentioning that only charge degrees of freedom appear in  $\mathcal{L}_0(\tau)$ , and spin degrees of freedom are now restricted to  $\mathcal{L}_n(\tau)$ , which includes both spin and charge dynamics intrinsically coupled.

### III. CHARGE DEGREES OF FREEDOM AND THE STRONG-COUPLING LIMIT

In this section, we shall first prove, that the Lagrangian  $\mathcal{L}_0(\tau)$  can be exactly diagonalized by a sequence of canonical transformations. Then, by introducing a perturbative expansion in the strong-coupling regime, a low-energy effective Lagrangian for the  $AB_2$  Hubbard chains in the half-filled and doped regimes will be obtained.

#### A. Charge degrees of freedom

We begin our discussion by considering the Lagrangian  $\mathcal{L}_0$  in Eq. (10), and its corresponding Hamiltonian  $\mathcal{H}_0$ , free of the spin-related vector fields  $\mathbf{n}_{i\alpha}$ . By performing the Legendre transformation:  $\mathcal{H}_0 = -\sum_{i\alpha\sigma} \frac{\partial \mathcal{L}_0}{\partial (\partial_\tau a_{i\alpha\sigma})} \partial_\tau a_{i\alpha\sigma} + \mathcal{L}_0$ , where  $\frac{\partial \mathcal{L}_0}{\partial (\partial_\tau a_{i\alpha\sigma})} = a_{i\alpha\sigma}^\dagger$ , the resulting  $\mathcal{H}_0$  is given by

$$\begin{aligned} \mathcal{H}_0 = & - \sum_{\langle i\alpha, j\beta \rangle \sigma} (t_{ij}^{\alpha\beta} a_{i\alpha\sigma}^\dagger a_{j\beta\sigma} + \text{H.c.}) \\ & + \frac{U}{2} \sum_{i\alpha\sigma} (1 - p_{i\alpha}\sigma) a_{i\alpha\sigma}^\dagger a_{i\alpha\sigma}. \end{aligned} \quad (12)$$

The special  $AB_2$  unit cell exhibit a symmetry<sup>10,12,25,26,43</sup> under the exchange of the labels of the  $B$  sites in a given unit cell. Thus, we can construct a new set of Grassmann fields possessing this symmetry, i.e., either symmetric or antisymmetric with respect to the exchange operation  $B_1 \leftrightarrow B_2$ , such as

$$\begin{aligned} d_{i\sigma} &= \frac{1}{\sqrt{2}}(a_{iB_1\sigma} + a_{iB_2\sigma}), \\ e_{i\sigma} &= \frac{1}{\sqrt{2}}(a_{iB_1\sigma} - a_{iB_2\sigma}), \\ b_{i\sigma} &= a_{iA\sigma}. \end{aligned} \quad (13)$$

Because we are interested in diagonalizing the equation (12) in the momentum space, it is useful to perform a Fourier transform for the above Grassmann fields as fol-

lows

$$\begin{aligned} d_{i\sigma} &= \frac{1}{\sqrt{N_c}} \sum_k e^{ikx_i} d_{k\sigma}, \\ e_{i\sigma} &= \frac{1}{\sqrt{N_c}} \sum_k e^{ikx_i} e_{k\sigma}, \\ b_{i\sigma} &= \frac{1}{\sqrt{N_c}} \sum_k e^{ikx_i} b_{k\sigma}, \end{aligned} \quad (14)$$

where  $k = 2\pi j(\frac{3}{N}) - \pi$ , with  $j = 1, \dots, N/3$ , and  $x_i = i$ , with  $i = 1, \dots, N/3$  is the position of the  $i$ th unit cell along the  $x$ -axis (where the length of the unit cell is set to unity). Then, we can rewrite  $\mathcal{H}_0$  as

$$\begin{aligned} \mathcal{H}_0 &= -\sqrt{2}t \sum_{k\sigma} (b_{k\sigma}^\dagger d_{k\sigma} + e^{ik} d_{k\sigma}^\dagger b_{k\sigma} + H.c) \\ &+ \frac{U}{2} \sum_{k\sigma} [(1+\sigma)b_{k\sigma}^\dagger b_{k\sigma} + (1-\sigma)(d_{k\sigma}^\dagger d_{k\sigma} + e_{k\sigma}^\dagger e_{k\sigma})], \end{aligned} \quad (15)$$

which is not a diagonal Hamiltonian, even for  $U = 0$ . As a signature of the quasi-1D structure of the  $AB_2$  chains, we notice that the  $B_1$  and  $B_2$  sites are located at a distance  $1/2$  (in the unit of length used) ahead of the  $A$  site. We can thus make use of this feature to properly introduce a phase factor  $e^{\frac{ik}{2}}$  through the following transformation<sup>43</sup>:

$$\begin{aligned} A_{k\sigma} &= \frac{1}{\sqrt{2}}(d_{k\sigma} + e^{\frac{ik}{2}} b_{k\sigma}), \\ B_{k\sigma} &= \frac{1}{\sqrt{2}}(d_{k\sigma} - e^{\frac{ik}{2}} b_{k\sigma}), \end{aligned} \quad (16)$$

and  $\mathcal{H}_0$  in Eq. (15) thus becomes

$$\begin{aligned} \mathcal{H}_0 &= \sum_{k\sigma} \varepsilon_k [A_{k\sigma}^\dagger A_{k\sigma} - B_{k\sigma}^\dagger B_{k\sigma}] + \frac{U}{2} \sum_{k\sigma} (1-\sigma) e_{k\sigma}^\dagger e_{k\sigma} \\ &+ \frac{U}{2} \sum_{k\sigma} [A_{k\sigma}^\dagger A_{k\sigma} + B_{k\sigma}^\dagger B_{k\sigma} - \sigma(A_{k\sigma}^\dagger B_{k\sigma} + B_{k\sigma}^\dagger A_{k\sigma})], \end{aligned} \quad (17)$$

where

$$\varepsilon_k = -2\sqrt{2}t \cos(k/2). \quad (18)$$

Lastly, we can exactly diagonalize  $\mathcal{H}_0$  through the following Bogoliubov transformation:

$$A_{k\sigma} = u_k \alpha_{k\sigma} - \sigma v_k \beta_{k\sigma}, \quad B_{k\sigma} = \sigma v_k \alpha_{k\sigma} + u_k \beta_{k\sigma}, \quad (19)$$

with  $u_k$  and  $v_k$  satisfying the canonical constraint:  $(u_k)^2 + (v_k)^2 = 1$ , so to maintain the fermionic anticommutation relations. Due to the ferrimagnetic order of the

GS, the above transformation is subject to a  $4\pi$  periodicity of the functions (fields)  $\{u_k, v_k\}$  and  $\{\alpha_{k\sigma}, \beta_{k\sigma}\}$ . The diagonalized  $\mathcal{H}_0$  thus reads:

$$\begin{aligned} \mathcal{H}_0 &= - \sum_{k\sigma} (E_k - \frac{U}{2}) \alpha_{k\sigma}^\dagger \alpha_{k\sigma} + \sum_{k\sigma} (E_k + \frac{U}{2}) \beta_{k\sigma}^\dagger \beta_{k\sigma} \\ &+ \frac{U}{2} \sum_{k\sigma} (1-\sigma) e_{k\sigma}^\dagger e_{k\sigma}, \end{aligned} \quad (20)$$

where

$$u_k = \frac{1}{\sqrt{2}} \left(1 + \frac{|\varepsilon_k|}{E_k}\right)^{1/2}, \quad v_k = \frac{1}{\sqrt{2}} \left(1 - \frac{|\varepsilon_k|}{E_k}\right)^{1/2}, \quad (21)$$

and

$$E_k = \sqrt{\varepsilon_k^2 + U^2/4}. \quad (22)$$

As one can see from Eq. (20), the non-interacting tight binding ( $U = 0$ ) spectrum of  $\mathcal{H}_0$  present three electronic bands: a nondispersive flat band (related to the Grassmann fields  $\{e_{k\sigma}^\dagger, e_{k\sigma}\}$ , macroscopically degenerate), and two dispersive ones. For  $AB_2$  chains, flat bands are closely associated with the ferrimagnetic properties at half filling<sup>8,18</sup>. The  $U = 0$  spin degeneracy of the flat bands is removed by the Coulombian repulsive interaction, in which case a gap  $U$  opens between the  $e_{k\sigma}$  modes:  $e_{k\uparrow} = 0$ , where spins at sites  $B_1$  and  $B_2$  are up, and  $e_{k\downarrow} = U$ , where spins at those sites are down. On the other hand, the two dispersive bands are spin degenerated, with a Hubbard gap  $U$ , separating the low ( $\alpha_{k\sigma}$ )-energy and high ( $\beta_{k\sigma}$ )-energy modes<sup>43</sup>.

## B. Strong-coupling limit

In this subsection, we shall introduce a perturbative expansion in the strong-coupling regime ( $U \gg t$ ) in order to obtain a low-energy effective Lagrangian for the  $AB_2$  Hubbard chain in the half-filled and doped regimes. Thereby, we first expand Eq. (21) in power of  $t/U$  as follows

$$\begin{aligned} u_k &\approx \frac{1}{\sqrt{2}} \left[ 1 + \frac{|\varepsilon_k|}{U} - \frac{|\varepsilon_k|^2}{2U^2} + \mathcal{O}\left(\frac{t^3}{U^3}\right) \right], \\ v_k &\approx \frac{1}{\sqrt{2}} \left[ 1 - \frac{|\varepsilon_k|}{U} - \frac{|\varepsilon_k|^2}{2U^2} + \mathcal{O}\left(\frac{t^3}{U^3}\right) \right]. \end{aligned} \quad (23)$$

Next, it will prove useful to define a set of auxiliary spinless Grassmann fields<sup>42,43</sup> in direct space as

$$\begin{aligned}\alpha_i &= \sqrt{\frac{1}{N_c}} \sum_{\sigma} \theta(\sigma) \sum_k e^{ikx_i} \alpha_{k\sigma}, \\ \beta_i &= \sqrt{\frac{1}{N_c}} \sum_{\sigma} \theta(-\sigma) \sum_k e^{ikx_i} \beta_{k\sigma}, \\ \alpha_i^{\frac{1}{2}} &= \sqrt{\frac{1}{N_c}} \sum_{\sigma} \theta(-\sigma) \sum_k e^{ikx_i} e^{-\frac{ik}{2}} \alpha_{k\sigma}, \\ \beta_i^{\frac{1}{2}} &= \sqrt{\frac{1}{N_c}} \sum_{\sigma} \theta(\sigma) \sum_k e^{ikx_i} e^{-\frac{ik}{2}} \beta_{k\sigma}, \\ e_{i,\sigma} &= \sqrt{\frac{1}{N_c}} \sum_k e^{ikx_i} e_{k,\sigma},\end{aligned}\quad (24)$$

where  $\theta(\sigma)$  is the Heaviside function and again, the phase factor  $e^{-\frac{ik}{2}}$  signalizes the quasi-1D  $AB_2$  structure. Now, by using the Eqs. (14), (16) and (19), we can write the Grassmann fields  $d_{i\sigma}$  and  $b_{i\sigma}$  in terms of the Bogoliubov fields  $\alpha_{k\sigma}$  and  $\beta_{k\sigma}$ :

$$d_{i\sigma} = \frac{1}{\sqrt{2N_c}} \sum_k e^{ikx_i} [(u_k + \sigma v_k) \alpha_{k\sigma} + (u_k - \sigma v_k) \beta_{k\sigma}], \quad (25)$$

$$b_{i\sigma} = \frac{1}{\sqrt{2N_c}} \sum_k e^{ik(x_i - \frac{1}{2})} [(u_k - \sigma v_k) \alpha_{k\sigma} - (u_k + \sigma v_k) \beta_{k\sigma}]. \quad (26)$$

Lastly, by substituting Eq. (23) into the Eqs. (25) and (26), and using the inverse transformation of (24), we can derive a perturbative expansion in powers of  $t/U$  for the Grassmann fields  $d_{i\sigma}$  and  $b_{i\sigma}$  in terms of the spinless Grassmann fields (24) up to order  $(t^2/U^2)$  as follows:

$$\begin{aligned}d_{i\sigma} &= \theta(\sigma) \alpha_i + \theta(-\sigma) \beta_i + \sqrt{2} \frac{t}{U} \theta(-\sigma) (\alpha_i^{\frac{1}{2}} + \alpha_{i+1}^{\frac{1}{2}}) \\ &\quad + \frac{t}{U} \theta(\sigma) [\sqrt{2} (\beta_i^{\frac{1}{2}} + \beta_{i+1}^{\frac{1}{2}}) - \frac{t}{U} (2\alpha_i + \alpha_{i+1} + \alpha_{i-1})] \\ &\quad - \frac{t^2}{U^2} \theta(-\sigma) (2\beta_i + \beta_{i+1} + \beta_{i-1}),\end{aligned}\quad (27)$$

$$\begin{aligned}b_{i\sigma} &= \theta(-\sigma) \alpha_i^{\frac{1}{2}} - \theta(\sigma) \beta_i^{\frac{1}{2}} + \sqrt{2} \frac{t}{U} \theta(\sigma) (\alpha_i + \alpha_{i-1}) \\ &\quad - \frac{t}{U} \theta(-\sigma) [\sqrt{2} (\beta_i + \beta_{i-1}) + \frac{t}{U} (2\alpha_i^{\frac{1}{2}} + \alpha_{i+1}^{\frac{1}{2}} + \alpha_{i-1}^{\frac{1}{2}})] \\ &\quad + \frac{t^2}{U^2} \theta(\sigma) (2\beta_i^{\frac{1}{2}} + \beta_{i+1}^{\frac{1}{2}} + \beta_{i-1}^{\frac{1}{2}}).\end{aligned}\quad (28)$$

In the above derivation we have used that  $\theta(\sigma)\theta(\sigma') = \theta(\sigma)\delta_{\sigma,\sigma'}$ . Notice that, since  $\frac{t}{U} \ll 1$  in Eqs. (27) and (28), we can identify the fields  $\alpha_i^{\frac{1}{2}} \approx a_{iA\downarrow}$  and  $\alpha_i \approx (a_{iB_1\uparrow} + a_{iB_2\uparrow})/\sqrt{2}$ , a result fully consistent with the low-energy spin configuration of the ferrimagnetic state discussed previously. Analogously, for the high-energy

bands, the opposite spin configuration is observed, with spin up (down) present at sites  $A$  ( $B_1, B_2$ ).

Introducing Eqs. (27) and (28) into Eq. (12), we obtain a perturbative expression for  $\mathcal{H}_0$  (low-energy sector) in terms of the spinless Grassmann fields up to order  $J = 4t^2/U$ :

$$\begin{aligned}\mathcal{H}_0 &= -J \sum_i [\alpha_i^\dagger \alpha_i + \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{\frac{1}{2}} - \beta_i^\dagger \beta_i - \beta_i^{(\frac{1}{2})\dagger} \beta_i^{\frac{1}{2}}] \\ &\quad + U \sum_i [\beta_i^\dagger \beta_i + \beta_i^{(\frac{1}{2})\dagger} \beta_i^{\frac{1}{2}} + e_{i\downarrow}^\dagger e_{i\downarrow}] - \frac{J}{2} \sum_i [\alpha_i^\dagger \alpha_{i+1} \\ &\quad + \alpha_i^{(\frac{1}{2})\dagger} \alpha_{i+1}^{\frac{1}{2}} - \beta_i^\dagger \beta_{i+1} - \beta_i^{(\frac{1}{2})\dagger} \beta_{i+1}^{\frac{1}{2}} + \text{H.c.}].\end{aligned}\quad (29)$$

In the above equation we note the presence of the band shrinking phenomenon<sup>8</sup>, in which case the width of the bands in the strong-coupling limit<sup>43</sup> is defined by  $J$ , whereas the U-dependent gap is opened between the low and high-energy bands. In order to describe the most relevant low-energy processes that take place in this regime, one has to additionally project out the high-energy bands from  $\mathcal{H}_0$ , that is, terms containing only fields related to the high-energy bands:  $\beta_i, \beta_i^{\frac{1}{2}}$  and  $e_{i\downarrow}^\dagger$ , are excluded. Therefore, after the Legendre transformation,  $\mathcal{H}_0 = -\sum_{i,\eta_i} \frac{\partial \mathcal{L}_0}{\partial (\partial_\tau \eta_i)} \partial_\tau \eta_i + \mathcal{L}_0$ , where  $\eta_i = \alpha_i, \alpha_i^{\frac{1}{2}}$  and  $e_{i\uparrow}$  (fields related to the low-energy bands), with  $\frac{\partial \mathcal{L}_0}{\partial (\partial_\tau \eta_i)} = \eta_i^\dagger$ , the Lagrangian associated with  $\mathcal{H}_0$ , up to order  $J$  is given by

$$\begin{aligned}\mathcal{L}_0 &= \sum_i [\alpha_i^\dagger \partial_\tau \alpha_i + \alpha_i^{(\frac{1}{2})\dagger} \partial_\tau \alpha_i^{\frac{1}{2}} + e_{i\uparrow}^\dagger \partial_\tau e_{i\uparrow}] \\ &\quad - J \sum_i [\alpha_i^\dagger \alpha_i + \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{\frac{1}{2}}] \\ &\quad - \frac{J}{2} \sum_i [\alpha_i^\dagger \alpha_{i+1} + \alpha_i^{(\frac{1}{2})\dagger} \alpha_{i+1}^{\frac{1}{2}} + \text{H.c.}].\end{aligned}\quad (30)$$

Next, we shall be interested in the  $U \gg t$  perturbative expansion of  $\mathcal{L}_n$ , Eq. (11), which amounts to consider the most significant low-energy processes. For the sake of clarity and completeness, the full derivation of the perturbative expansion of  $\mathcal{L}_n$  is given in the Appendix. Here we restrict ourselves to present only the final result. Indeed, by adding  $\mathcal{L}_0$  to the perturbative expansion of  $\mathcal{L}_n$ , the effective low-energy Lagrangian density of the  $AB_2$  Hubbard model in the strong-coupling limit (up to order  $J$ ) reads:

$$\mathcal{L}_{eff}(\tau) = \mathcal{L}^{(I)} + \mathcal{L}^{(II)} + \mathcal{L}^{(III)} + \mathcal{L}^{(IV)}, \quad (31)$$

where

$$\mathcal{L}^{(I)} = \sum_i \alpha_i^\dagger \partial_\tau \alpha_i + \sum_i \alpha_i^{(\frac{1}{2})\dagger} \partial_\tau \alpha_i^{\frac{1}{2}} + \sum_i e_{i\uparrow}^\dagger \partial_\tau e_{i\uparrow}, \quad (32a)$$



$$\begin{aligned}\mathcal{L}^{(II)} = & \sum_{i\sigma} \left\{ \theta(-\sigma) (U_i^{(b)\dagger} \partial_\tau U_i^{(b)})_{\sigma,\sigma} \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})} \right. \\ & + \theta(\sigma) \frac{1}{2} [(U_i^{(d)\dagger} \partial_\tau U_i^{(d)})_{\sigma,\sigma} + (U_i^{(e)\dagger} \partial_\tau U_i^{(e)})_{\sigma,\sigma}] \\ & \times (\alpha_i^\dagger \alpha_i + e_{i\uparrow}^\dagger e_{i\uparrow}) + \left[ \theta(\sigma) \frac{1}{2} [(U_i^{(d)\dagger} \partial_\tau U_i^{(e)})_{\sigma,\sigma} \right. \\ & \left. \left. + (U_i^{(e)\dagger} \partial_\tau U_i^{(d)})_{\sigma,\sigma}] \alpha_i^\dagger e_{i\uparrow} + \text{H.c.} \right] \right\}, \quad (32b)\end{aligned}$$

$$\begin{aligned}\mathcal{L}^{(III)} = & -t \sum_{i\sigma} \left\{ \theta(-\sigma) (U_i^{(b)\dagger} U_i^{(d)})_{\sigma,-\sigma} \alpha_i^{(\frac{1}{2})\dagger} \alpha_i \right. \\ & + \theta(\sigma) (U_i^{(d)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} \alpha_i^\dagger \alpha_{i+1}^{(\frac{1}{2})} \\ & + \theta(-\sigma) (U_i^{(b)\dagger} U_i^{(e)})_{\sigma,-\sigma} \alpha_i^{(\frac{1}{2})\dagger} e_{i\uparrow} \\ & \left. + \theta(\sigma) (U_i^{(e)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} e_{i\uparrow}^\dagger \alpha_{i+1}^{(\frac{1}{2})} + \text{H.c.} \right\}, \quad (32c)\end{aligned}$$

$$\begin{aligned}\mathcal{L}^{(IV)} = & -\frac{J}{4} \sum_{i;i'=i,i+1;\sigma} \theta(\sigma) |(U_i^{(d)\dagger} U_{i'}^{(b)})_{\sigma,\sigma}|^2 \alpha_i^\dagger \alpha_i \\ & -\frac{J}{4} \sum_{i;i'=i,i+1;\sigma} \theta(\sigma) |(U_i^{(e)\dagger} U_{i'}^{(b)})_{\sigma,\sigma}|^2 e_{i\uparrow}^\dagger e_{i\uparrow} \\ & -\frac{J}{4} \sum_{i;i'=i,i-1;\sigma} \theta(-\sigma) |(U_i^{(b)\dagger} U_{i'}^{(d)})_{\sigma,\sigma}|^2 \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})} \\ & -\frac{J}{4} \sum_{i;i'=i,i-1;\sigma} \theta(-\sigma) |(U_i^{(b)\dagger} U_{i'}^{(e)})_{\sigma,\sigma}|^2 \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})}. \quad (32d)\end{aligned}$$

From the above equations, we see that the kinetic term is represented by  $\mathcal{L}^{(I)}$  and is related to the charge degrees of freedom only, whereas  $\mathcal{L}^{(II)}$  describes the dynamics of the spin degrees of freedom coupled to the charge fields. On the other hand,  $\mathcal{L}^{(III)}$  exhibit first-neighbor hopping contributions between charge degrees of freedom in the presence of spin gauge fields, while  $\mathcal{L}^{(IV)}$  is the spin exchange term in the presence of the charge Grassmann fields.

#### IV. HALF FILLING REGIME

Let us now discuss some basic aspects of the localized magnetic properties related to the spin degrees of freedom. At half filling, i.e.,  $\delta = 0$ , where  $\delta$  represents hole doping, we have  $\langle \alpha_i^\dagger \alpha_i \rangle = 1$ ,  $\langle \alpha_i^{(1/2)\dagger} \alpha_i^{(1/2)} \rangle = 1$ ,  $\langle e_{i\uparrow}^\dagger e_{i\uparrow} \rangle = 1$ , and  $\langle \alpha_i^\dagger e_{i\uparrow} \rangle = 0$  (no band hybridization) as the electrons tend to fill up the lower-energy bands, whereas the higher-energy ones remain empty. As a consequence, a ferrimagnetic configuration of localized spin emerges, i.e., the charge degrees of freedom are completely frozen, such that  $\langle \alpha_i^\dagger \partial_\tau \alpha_i \rangle = \langle \alpha_i^{(1/2)\dagger} \partial_\tau \alpha_i^{(1/2)} \rangle = \langle e_{i\uparrow}^\dagger \partial_\tau e_{i\uparrow} \rangle = 0$ , with forbidden hopping. Therefore, only

terms from  $\mathcal{L}^{II}$  and  $\mathcal{L}^{IV}$  in Eqs. (32b) and (32d), respectively, give nonzero contributions and the resulting effective strong-coupling Lagrangian at half filling reads:

$$\begin{aligned}\mathcal{L}_{eff} = & \sum_{i\alpha\sigma} \theta(p_{i\alpha}\sigma) (U_{i\alpha}^\dagger \partial_\tau U_{i\alpha})_{\sigma,\sigma} \\ & -\frac{J}{4} \sum_{\langle i\alpha,j\beta \rangle \sigma} \theta(p_{i\alpha}\sigma) \left| (U_{i\alpha}^\dagger U_{j\beta})_{\sigma,\sigma} \right|^2. \quad (33)\end{aligned}$$

where the staggered factor  $p_{i\alpha}$  was defined in Sec. (II), and use was made of the matrix transformations defined in Eq. (A.1). Now, using the following Legendre transform:

$$\mathcal{H}_{eff} = -\sum_{i\alpha\sigma} \frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau U_{i\alpha})_{\sigma,\sigma}} (\partial_\tau U_{i\alpha})_{\sigma,\sigma} + \mathcal{L}_{eff}, \quad (34)$$

where  $\frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau U_{i\alpha})_{\sigma,\sigma}} = \theta(p_{i\alpha}\sigma) (U_{i\alpha}^\dagger)_{\sigma,\sigma}$ , we get the respective quantum Heisenberg Hamiltonian written in terms of the  $SU(2)$  gauge fields at half filling as

$$\mathcal{H}_{eff}^J = -\frac{J}{4} \sum_{\langle i\alpha,j\beta \rangle \sigma} \theta(p_{i\alpha}\sigma) \left| (U_{i\alpha}^\dagger U_{j\beta})_{\sigma,\sigma} \right|^2. \quad (35)$$

Further, using the definition of the  $SU(2)/U(1)$  unitary rotation matrix Eq. (7), it is possible to write<sup>42–44</sup>  $\left| (U_{i\alpha}^\dagger U_{j\beta})_{\sigma,\sigma} \right|^2 = \frac{1}{2} (1 + \mathbf{n}_{i\alpha} \cdot \mathbf{n}_{j\beta})$ , where  $\mathbf{n}_{i\alpha} = \sin(\theta_{i\alpha}) [\cos(\phi_{i\alpha}) \hat{\mathbf{x}} + \sin(\phi_{i\alpha}) \hat{\mathbf{y}}] + \cos(\theta_{i\alpha}) \hat{\mathbf{z}}$  is the local unit vector, and thereby Eq. (35) takes the form

$$\begin{aligned}\mathcal{H}_{eff}^J = & -\frac{J}{4} \sum_i \{ 4 + \mathbf{n}_{iA} \cdot (\mathbf{n}_{iB_1} + \mathbf{n}_{iB_2}) \\ & + (\mathbf{n}_{iB_1} + \mathbf{n}_{iB_2}) \cdot \mathbf{n}_{i+1A} \}. \quad (36)\end{aligned}$$

Lastly, using  $\mathbf{S}_{i\alpha} = \mathbf{n}_{i\alpha}/2$ , we obtain

$$\mathcal{H}_{eff}^J = -J \sum_i \left[ (\mathbf{S}_{iB_1}^{B_1} + \mathbf{S}_{iB_2}^{B_2}) \cdot (\mathbf{S}_i^A + \mathbf{S}_{i+1}^A) \right] - JN_c. \quad (37)$$

The above expression is indeed that of the quantum Heisenberg model on the  $AB_2$  chain in zero-field. Now, we are interested in gain a better understanding of the quantum Heisenberg model on  $AB_2$  chains, particularly its GS energy, taking into account the effects of zero-point quantum spin fluctuations. In fact, we analyze the Hamiltonian, Eq. (37), by means of the spin-wave theory, which has proved very successful in describing the properties of the GS and low-lying excited states of spin models. To achieve this goal, we shall first introduce boson creation and annihilation operators via the Holstein-Primakoff<sup>49</sup> transformation:

$$\begin{aligned}S_i^{A,z} &= -S + a_i^\dagger a_i, \\ S_i^{A,+} &= (S_i^{A,-})^\dagger = \sqrt{2S} a_i^\dagger f_A(S), \quad (38)\end{aligned}$$

for a down-spin on the  $A$  site, and

$$\begin{aligned} S_i^{B_l, z} &= S - b_{li}^\dagger b_{li}, \\ S_i^{B_l, +} &= (S_i^{B_l, -})^\dagger = \sqrt{2S} f_B(S) b_{li}, \end{aligned} \quad (39)$$

for an up-spin on the  $B_l$  site, with  $l = 1, 2$ , and

$$f_r(S) = \left(1 - \frac{n_r}{2S}\right)^{1/2} = 1 - \frac{1}{2} \frac{n_r}{2S} + \dots, \quad (40)$$

where  $S$  is the spin magnitude, and  $n_r = a_i^\dagger a_i$  or  $b_{li}^\dagger b_{li}$ . The operators  $a_i^\dagger$  and  $a_i$  (or  $b_{li}^\dagger$ ,  $b_{li}$ ) satisfy the boson commutation rules  $[a_i, a_{i'}^\dagger] = \delta_{ii'}$ . Under the above transformation, the spin Hamiltonian, Eq. (37) is mapped onto the equivalent boson Hamiltonian:

$$\mathcal{H}_{eff}^J = E_0 + \mathcal{H}_1 + \mathcal{H}_2 - JN_c + \mathcal{O}(S^{-1}), \quad (41)$$

where

$$\begin{aligned} \mathcal{H}_1 &= 2JS \sum_i \left( 2a_i^\dagger a_i + \sum_{l=1,2} b_{li}^\dagger b_{li} \right) \\ &+ JS \sum_{i,l} \left( a_i^\dagger b_{li}^\dagger + a_i b_{li} + b_{li}^\dagger a_{i+1}^\dagger + b_{li} a_{i+1} \right), \end{aligned} \quad (42)$$

and

$$\begin{aligned} \mathcal{H}_2 &= -J \sum_{i,l} \left( a_i^\dagger a_i b_{li}^\dagger b_{li} + a_{i+1}^\dagger a_{i+1} b_{li}^\dagger b_{li} \right) \\ &- \frac{J}{4} \sum_{i,l} \left( a_i^\dagger b_{li}^\dagger b_{li}^\dagger b_{li} + a_{i+1}^\dagger b_{li}^\dagger b_{li}^\dagger b_{li} \right. \\ &\left. + a_i^\dagger a_i^\dagger a_i b_{li}^\dagger + a_{i+1}^\dagger a_{i+1}^\dagger a_{i+1} b_{li}^\dagger + \text{H.c.} \right). \end{aligned} \quad (43)$$

Above,  $E_0 = -4S^2 JN_c$ ,  $\mathcal{H}_1$  and  $\mathcal{H}_2$  represent the classical GS energy, the quadratic and quartic interacting terms of the boson Hamiltonian, with orders  $\mathcal{O}(S^2)$ ,  $\mathcal{O}(S^1)$  and  $\mathcal{O}(S^0)$ , respectively, suitable to describe the properties of the quantum  $AB_2$  Heisenberg model, via a perturbative series expansion in powers of  $1/S$ .

Now, we introduce the Bloch-type operator  $a_k$ ,  $b_{lk}$  (satisfying the boson commutation rules  $[a_k, a_{k'}^\dagger] = \delta_{kk'}$ ) through the Fourier transformation

$$a_i = \sqrt{\frac{3}{N}} \sum_k e^{ikx_i} a_k, \quad b_{li} = \sqrt{\frac{3}{N}} \sum_k e^{-ik(x_i + \frac{1}{2})} b_{lk}, \quad (44)$$

where  $k$  varies over  $N/3$  wave vectors in the first Brillouin zone, and  $e^{-\frac{ik}{2}}$  is the phase factor introduced in Eq. (16). Thus, the quadratic boson Hamiltonian is then given by

$$\begin{aligned} \mathcal{H}_1 &= 2JS \sum_k \left( 2a_k^\dagger a_k + \sum_l b_{lk}^\dagger b_{lk} \right) \\ &+ \sum_{k,l=1,2} 2JS \gamma_k \left( a_k^\dagger b_{lk}^\dagger + a_k b_{lk} \right), \end{aligned} \quad (45)$$

where we have defined the lattice structure factor as

$$\gamma_k = \frac{1}{z} \sum_\rho e^{ik\rho} = \cos\left(\frac{k}{2}\right), \quad (46)$$

with  $z$  denoting the coordination number ( $z = 4$  for the  $AB_2$  chain), while  $\rho = \pm 1/2$  connects the nearest neighbors  $A$ - $B_1$  and  $A$ - $B_2$  linked sites of sublattices  $A$  and  $B$ , and

$$\begin{aligned} \mathcal{H}_2 &= -\frac{3J}{2N} \sum_{1234, l=1,2} \delta_{12,34} \left\{ 4\gamma_{1-4} a_1^\dagger a_4 b_{l3}^\dagger b_{l2} \right. \\ &\left. + \left( \gamma_1 a_1^\dagger b_{l4}^\dagger b_{l3}^\dagger b_{l2} + \gamma_{1+2-3} a_1^\dagger a_2^\dagger a_3 b_{l4}^\dagger + \text{H.c.} \right) \right\}, \end{aligned} \quad (47)$$

is the quartic boson interacting Hamiltonian in momentum space. We use the convention 1 for  $k_1$ , 2 for  $k_2$ , and so on. Also, the  $\delta_{12,34} = \delta(k_1 + k_2 - k_3 - k_4)$  is the Kronecker  $\delta$  function, and expresses the conservation of momentum to within a reciprocal-lattice vector  $G$ .

For now, we focus on  $\mathcal{H}_1$ , which is the only term considered in linear spin-wave theory (LSWT). To leading order, we can diagonalize the quadratic boson Hamiltonian  $\mathcal{H}_1$  by the following Bogoliubov transformations

$$\begin{aligned} a_k &= u_k \beta_k - v_k \alpha_k^\dagger, \\ b_{1,2k} &= \frac{1}{\sqrt{2}} \left( u_k \alpha_k - v_k \beta_k^\dagger \mp \xi_k \right), \end{aligned} \quad (48)$$

where

$$u_k = \frac{3 + \sqrt{9 - 8\gamma_k^2}}{\sqrt{\left(3 + \sqrt{9 - 8\gamma_k^2}\right)^2 - 8\gamma_k^2}}, \quad (49)$$

$$v_k = \frac{2\sqrt{2}\gamma_k}{\sqrt{\left(3 + \sqrt{9 - 8\gamma_k^2}\right)^2 - 8\gamma_k^2}}, \quad (50)$$

satisfy the constrain  $u_k^2 - v_k^2 = 1$ . After this transformation, we obtain

$$\mathcal{H}_1 = E_1 + \sum_k \left( \epsilon_k^{(\alpha)} \alpha_k^\dagger \alpha_k + \epsilon_k^{(\beta)} \beta_k^\dagger \beta_k + \epsilon_k^{(\xi)} \xi_k^\dagger \xi_k \right), \quad (51)$$

where  $\epsilon_k^{(\alpha, \beta)} = JS \left( \sqrt{9 - 8\gamma_k^2} \mp 1 \right)$ ,  $\epsilon_k^{(\xi)} = 2JS$  are the three spin-wave branches provided by LSWT, and  $E_1 = JS \sum_k \left( \sqrt{9 - 8\gamma_k^2} - 3 \right)$  is the zero-point energy, i.e., the  $\mathcal{O}(S^1)$  quantum correction to the GS energy, in agreement with previous results<sup>20,50</sup>. In fact, it is well known that systems with a ferrimagnetic GS naturally have ferromagnetic and antiferromagnetic spin-wave modes as their elementary magnetic excitations (magnons)<sup>6,51</sup>. For the  $AB_2$  chain, there are three spin-wave branches: an antiferromagnetic mode ( $\epsilon_k^{(\beta)}$ ) and two ferromagnetic ones ( $\epsilon_k^{(\alpha)}$  and  $\epsilon_k^{(\xi)}$ ). The mode  $\epsilon_k^{(\alpha)}$  is gapless at  $k = 0$ , i.e., the Goldstone mode, with a quadratic

(ferromagnetic) dispersion relation  $\epsilon_k^{(\alpha)} \sim k^2$ . The other two modes are gapped. Notice that the gapped ferromagnetic mode  $\epsilon_k^{(\xi)}$  is flat, and is closely associated with ferrimagnetic properties at half filling<sup>8,18</sup>. Since the dispersive modes preserve the local triplet bond, they are identical to those found in the spin- $\frac{1}{2}$ /spin-1 chain<sup>51-53</sup>.

### A. Analysis of the interaction Hamiltonian

There exist many ways of dealing with the bosonic quartic interactions in Eq. (47)<sup>51,53-57</sup>. Here, our aim is to obtain the leading corrections to LSWT, i.e., second-order spin-wave theory, to the GS energy, dispersion relations, and sublattice magnetizations. In doing so, we develop a perturbative scheme for the description of this quartic term. First, we decompose the two-body terms by means of the Wick theorem, via normal-ordering protocol for boson operators. Conservation of momentum to within a reciprocal-lattice vector, implies:  $k_1 = k + q$ ,  $k_2 = p - q$ ,  $k_3 = k$  and  $k_4 = p$ , in Eq. (43). Then, we need to look at the possible pairings of the 4 operators, as for example, the first term of Eq. (47):

$$a_{k+q}^\dagger a_p b_{l,k}^\dagger b_{l,p-q}, \quad a_{k+q}^\dagger a_p b_{l,k}^\dagger b_{l,p-q}, \quad a_{k+q}^\dagger a_p b_{l,k}^\dagger b_{l,p-q}.$$

Under this procedure, substituting the Bogoliubov transformation, Eq. (48), and normal ordering the terms, we finally obtain

$$\mathcal{H}_2 = E_2 + J \sum_k \left( \delta\epsilon_k^{(\alpha)} \alpha_k^\dagger \alpha_k + \delta\epsilon_k^{(\beta)} \beta_k^\dagger \beta_k + \delta\epsilon_k^{(\xi)} \xi_k^\dagger \xi_k \right), \quad (52)$$

where

$$E_2 = -\frac{2J}{N_c} \left( \sum_k v_k^2 \right)^2 - \frac{2J}{N_c} \left( \sum_k \gamma_k u_k v_k \right)^2 + \frac{3\sqrt{2}J}{N_c} \sum_k (v_k^2) \sum_p (\gamma_p u_p v_p) + \mathcal{O}(S^{-1}), \quad (53)$$

and the corresponding corrections for the dispersion relations read:  $E_k^s = J\omega_k^{(s)}$ , where  $\omega_k^{(s)} = \epsilon_k^{(s)} + \delta\epsilon_k^{(s)}$ , with  $s = \alpha, \beta, \xi$ , and

$$\delta\epsilon_k^{(\alpha)} = u_k^2 \left[ \sqrt{2}q_2 - 2q_1 \right] + 2v_k^2 \left[ \sqrt{2}q_2 - q_1 \right] + 4\gamma_k u_k v_k \left[ \frac{3}{2\sqrt{2}}q_1 - q_2 \right] + \mathcal{O}(S^{-1}), \quad (54)$$

$$\delta\epsilon_k^{(\beta)} = v_k^2 \left[ \sqrt{2}q_2 - 2q_1 \right] + 2u_k^2 \left[ \sqrt{2}q_2 - q_1 \right] + 4\gamma_k u_k v_k \left[ \frac{3}{2\sqrt{2}}q_1 - q_2 \right] + \mathcal{O}(S^{-1}), \quad (55)$$

$$\delta\epsilon_k^{(\xi)} = \sqrt{2}q_2 - 2q_1 + \mathcal{O}(S^{-1}), \quad (56)$$

with the definitions:

$$q_1 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk (v_k^2), \quad q_2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk (\gamma_k u_k v_k). \quad (57)$$

In deriving Eq. (53), we have neglected terms containing anomalous products, such as  $\alpha_k^\dagger \beta_k^\dagger$  and vertex corrections. The LSWT predicts a gap  $\Delta_{flat} = J$  for the flat mode ( $\omega_k^{(\xi)}$ ), whereas our second-order spin-wave theory<sup>20</sup> finds  $\Delta_{flat} = (1 - 2q_1 + \sqrt{2}q_2)J \simeq 1.066J$ . Surprisingly, the estimated value from ED<sup>6</sup>:  $\Delta_{flat} = 1.0004J$ , lies between these two theoretical values. On the other hand, our approach is able to improve the LSWT result for the gap  $\Delta = J$  of the antiferromagnetic mode ( $\omega_k^{(\beta)}$  at  $k = 0$ ), which should be compared with the corresponding result:  $\Delta = (1 + \sqrt{2}q_2)J \simeq 1.676J$ , of our perturbative  $1/S$  series expansion, in agreement with Ref. (52). The numerical estimation for the gap of the antiferromagnetic mode is  $\Delta = 1.759J$ <sup>6,52,53</sup>. On the other hand, to the best of our knowledge, analytical approaches based on spin-wave theories are still unable to reproduce the observed level crossing found in numerical calculations<sup>6,20</sup> for the two ferromagnetic modes. This is probably due to the fact that the distinct symmetries exhibited by both the localized excitation (flat mode) and the ferromagnetic dispersive mode are not properly considered in the analytical approach, as yet.

### B. Ground state energy

Now, we present the analytical results for the GS energy of the quantum Heisenberg model on  $AB_2$  chains. From the above results, the resultant effective Hamiltonian can be compactly represented as

$$\mathcal{H}_{eff} = E_{GS} + J \sum_k (\omega_k^\alpha \alpha_k^\dagger \alpha_k + \omega_k^{(\beta)} \beta_k^\dagger \beta_k + \omega_k^{(\xi)} \xi_k^\dagger \xi_k), \quad (58)$$

where the second-order spin-wave result up to  $\mathcal{O}(1/S)$  for the GS energy is  $E_{GS}^J = E_0 + E_1 + E_2$ . Therefore, in the thermodynamic limit, the GS energy per unit cell reads:

$$\frac{E_{GS}^J}{N_c} = -4JS^2 + \frac{JS}{2\pi} \int_{-\pi}^{\pi} dk \left( \sqrt{9 - 8\gamma_k^2} - 3 \right) - 2J \left( q_1^2 + q_2^2 - \frac{3}{\sqrt{2}}q_1 q_2 \right). \quad (59)$$

We remark that we shall not consider the last (constant) term in Eq. (41), since it introduces only a shift in the energy level, with the purpose of comparison with preceding results obtained for the GS energy of quantum  $AB_2$  Heisenberg model. Performing the integration over the first Brillouin zone (BZ) and taking  $S = 1/2$ , we obtain that the GS energy per site at zero-field is given by  $-0.4869J$ . This result agree very well with values obtained by using exact diagonalization<sup>38</sup> ( $-0.485J$ ) and



DMRG<sup>58</sup> ( $-0.4847J$ ) techniques. For the spin- $\frac{1}{2}$ /spin-1 chain, the value obtained using DMRG<sup>59</sup> is  $-0.72704J$ . To compare with our finding, we need to multiply this value by  $2/3$  (as the number of sites of this chain is exactly  $2/3$  of the  $AB_2$  chain), yielding  $-0.48469J$ .

### C. Sublattice magnetizations and Lieb GS total spin per unit cell

The sublattice magnetizations are defined by the GS expectation values:  $m_A = \langle \sum_{i=1}^{N_c} S_i^{A,z} \rangle$  and  $m_{B_l} = \langle \sum_{i=1}^{N_c} S_i^{B_l,z} \rangle$ . In order to derive results beyond LSWT, we introduce staggered magnetic fields coupled to spins  $S_i^{A,z}$  and  $S_i^{B_l,z}$  through the Zeeman terms:  $-h_A \sum_i S_i^{A,z}$  and  $-h_{B_l} \sum_i S_i^{B_l,z}$ , which are added to  $\mathcal{H}_{eff}^J$  in Eq. (37). Thus,  $m_A$  is obtained from  $m_A = -(1/N_c) \sum_{i=1,2} [\partial E_i(h_A)/\partial h_A]|_{h_A=0}$ , which reads:

$$m_A = -S + \frac{1}{2\pi} \int_{-\pi}^{\pi} dk v_k^2 - \left( \frac{1}{2S} \right) \frac{q_1}{\pi} \int_{-\pi}^{\pi} dk \frac{\gamma_k^2}{(9 - 8\gamma_k^2)^{3/2}} + \mathcal{O}\left(\frac{1}{S^2}\right). \quad (60)$$

Analogously, we find

$$m_{B_{1,2}} = S - \frac{1}{4\pi} \int_{-\pi}^{\pi} dk v_k^2 + \left( \frac{1}{2S} \right) \frac{q_1}{2\pi} \int_{-\pi}^{\pi} dk \frac{\gamma_k^2}{(9 - 8\gamma_k^2)^{3/2}} + \mathcal{O}\left(\frac{1}{S^2}\right). \quad (61)$$

Carrying out the above integration, we obtain  $m_A = -0.316343$  and  $m_{B_l} = 0.408172$ . These results are in good agreement with those obtained using DMRG<sup>12</sup> and ED<sup>6</sup> techniques:  $\langle S_i^{A,z} \rangle = -0.2925$  and  $\langle S_i^{B_l,z} \rangle = 0.3962$ , respectively, and with values for  $\langle S_i^{A,z} \rangle$  and  $2 \langle S_i^{B_l,z} \rangle$  for the spin- $\frac{1}{2}$ /spin-1 chain<sup>51-53</sup>. Although at zero temperature, the sublattice magnetizations are strongly reduced by quantum fluctuations, as compared with their classical values, the unit cell magnetization remains  $S_L \equiv 1/2$ , where  $S_L$  is the Lieb GS total spin per unit cell, in full agreement with Lieb's theorem<sup>16</sup> for bipartite lattices:

$$S_L = \frac{1}{2} \|N_A - N_B\|, \quad (62)$$

with  $N_A(N_B)$  denoting the total number of spins in sublattice  $A(B)$  per unit cell.

### V. $t$ - $J$ HAMILTONIAN: GROUND STATE ENERGY AND TOTAL SPIN

In this section, we shall derive the corresponding  $t$ - $J$  Hamiltonian suitable to describe the strongly correlated

$AB_2$  Hubbard chain in the doped regime, in which case both charge (Grassmann fields) and spin ( $SU(2)$  gauge fields) quantum fluctuations are considered on an equal footing. Indeed, the  $t$ - $J$  Hamiltonian can be derived by means of the following Legendre transformation to Eq. (31):

$$\mathcal{H}_{eff}^{t-J} = - \sum_{i,\mu=b,d,e} \frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau U_i^{(\mu)})_{\sigma,\sigma}} (\partial_\tau U_i^{(\mu)})_{\sigma,\sigma} - \sum_{i,\nu_i} \frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau \nu_i)} \partial_\tau \nu_i + \mathcal{L}_{eff}, \quad (63)$$

where

$$\frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau \nu_i)} = \nu_i^\dagger, \quad \text{with } \nu_i = \alpha_i, \alpha_i^{\frac{1}{2}}, e_{i\uparrow}, \quad (64)$$

and

$$\frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau U_i^{(b)})_{\sigma,\sigma}} = \theta(-\sigma) (U_i^{(b)\dagger})_{\sigma,\sigma} \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})}, \quad (65)$$

$$\frac{\partial \mathcal{L}_{eff}}{\partial (\partial_\tau U_i^{(d,e)})_{\sigma,\sigma}} = \theta(\sigma) \frac{1}{2} [(U_i^{(d,e)\dagger})_{\sigma,\sigma} (\alpha_i^\dagger \alpha_i + e_{i\uparrow}^\dagger e_{i\uparrow}) + (U_i^{(e,d)\dagger})_{\sigma,\sigma} (\alpha_i^\dagger e_{i\uparrow} + e_{i\uparrow}^\dagger \alpha_i)], \quad (66)$$

now, we can write the effective  $t$ - $J$  Hamiltonian as

$$\mathcal{H}_{eff}^{t-J} = \mathcal{H}^t + \mathcal{H}^J, \quad (67)$$

where

$$\begin{aligned} \mathcal{H}^t = & -t \sum_{i\sigma} \{ \theta(-\sigma) (U_i^{(b)\dagger} U_{i+1}^{(d)})_{\sigma,-\sigma} \alpha_i^{(1/2)\dagger} \alpha_i \\ & + \theta(\sigma) (U_i^{(d)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} \alpha_i^\dagger \alpha_{i+1}^{(1/2)} \\ & + \theta(-\sigma) (U_i^{(b)\dagger} U_{i+1}^{(e)})_{\sigma,-\sigma} \alpha_i^{(1/2)\dagger} e_{i\uparrow} \\ & + \theta(\sigma) (U_i^{(e)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} e_{i\uparrow}^\dagger \alpha_{i+1}^{(1/2)} + \text{H.c.} \}, \end{aligned} \quad (68)$$

and

$$\begin{aligned} \mathcal{H}^J = & -\frac{J}{4} \sum_{i;i'=i,i+1;\sigma} \theta(\sigma) |(U_i^{(d)\dagger} U_{i'}^{(b)})_{\sigma,\sigma}|^2 \alpha_i^\dagger \alpha_i \\ & -\frac{J}{4} \sum_{i;i'=i,i+1;\sigma} \theta(\sigma) |(U_i^{(e)\dagger} U_{i'}^{(b)})_{\sigma,\sigma}|^2 e_{i\uparrow}^\dagger e_{i\uparrow} \\ & -\frac{J}{4} \sum_{i;i'=i,i-1;\sigma} \theta(-\sigma) |(U_i^{(b)\dagger} U_{i'}^{(d)})_{\sigma,\sigma}|^2 \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})} \\ & -\frac{J}{4} \sum_{i;i'=i,i-1;\sigma} \theta(-\sigma) |(U_i^{(b)\dagger} U_{i'}^{(e)})_{\sigma,\sigma}|^2 \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})}. \end{aligned} \quad (69)$$

Notice that Eqs. (68) and (69) are identical to Eqs. (32c) and (32d), since Eqs. (32a) and (32b) were eliminated through the Legendre transformation. One of the key

properties of quasi-1D interacting quantum systems is the phenomenon of spin-charge separation, leading to the formation of spin and charge-density waves, which move independently and with different velocities. It has been demonstrated<sup>25</sup> that for  $\delta > 2/3$  the low-energy physics of the doped  $AB_2$  Hubbard chain in the  $U = \infty$  coupling limit is described in terms of the Luttinger-liquid model, with the spin and charge degrees of freedom decoupled. Most importantly recently it has been shown that for the  $AB_2$   $t$ - $J$  Hubbard chains<sup>26</sup>, charge and spin quantum fluctuations are practically decoupled, as suggested by the emergence of charge-density waves in anti-phase with the modulation of the ferrimagnetic order. One can make use of this property to formally split the  $t$ - $J$  Hamiltonian of the system into a product of two independent terms acting on different Hilbert spaces, i.e., we can enforce spin-charge separation and calculate the charge and spin correlation functions in a decoupled fashion. In order to proceed with the calculations, it is important to establish the regime of relevance to our model. We focus on the underdoped regime and values of  $J > 0$ , where electrons tend to become itinerant. In this regime, the formation of ferromagnetic polarons, a signature of Nagaoka phenomenon, is strongly reduced for not very low values of  $J$ . Therefore, we shall consider that the charge correlation function is described by the spinless tight-binding

model<sup>25,43,60</sup>:  $\langle \alpha_i^{(1/2)\dagger} \alpha_i \rangle = \langle \alpha_i^\dagger \alpha_{i+1}^{(1/2)} \rangle = \frac{2}{\pi} \sin(\frac{k_F}{2})$ ,  $\langle \alpha_i^{(1/2)\dagger} e_{i\uparrow} \rangle = 0$ , and thereby

$$\begin{aligned} \mathcal{H}_{eff}^{t-J} = & -t \frac{2}{\pi} \sin(\frac{k_F}{2}) \sum_{i\sigma} \{ (U_i^{(b)\dagger} U_i^{(d)})_{\downarrow\uparrow} \\ & + (U_i^{(d)\dagger} U_{i+1}^{(b)})_{\uparrow\downarrow} + \text{H.c.} \} \\ & - \frac{J(1-\delta)}{4} \sum_{\langle i\alpha, j\beta \rangle \sigma} \theta(p_{i\alpha}\sigma) |(U_{i\alpha}^\dagger U_{j\beta})_{\sigma,\sigma}|^2, \end{aligned} \quad (70)$$

where  $k_F$  is the Fermi wave vector. Here, we remark that the itinerant holes away from half filling (spinless fermions) are associated with the lower-energy dispersive  $\alpha_k$  band<sup>25,43</sup>: therefore,  $k_F = \pi \frac{N_h}{N_c}$ , where  $N_h$  is the number of holes. On the other hand, in real space the hole doping is given by  $\delta = N_h/2N_c$ , which implies  $k_F = 2\pi\delta$ , where  $2N_c$  is the number of sites of the effective linear chain, where holes (charge) density waves develop (along the  $x$ -axis) in anti-phase with the modulation of the ferrimagnetic structure, as numerically observed [see Fig. 2(b) of Ref. (26)].

We are now ready to examine in more detail some aspects of the spin sector in Eq. (70). The matrix elements:  $(U_i^{(b)\dagger} U_i^{(d)})_{\downarrow\uparrow}$  and  $(U_i^{(d)\dagger} U_{i+1}^{(b)})_{\uparrow\downarrow}$ , which are described by the  $SU(2)$  gauge fields, are written in terms of the spin fields<sup>43,44</sup> as

$$(U_i^{(b)\dagger} U_i^{(d)})_{\downarrow\uparrow} + \text{H.c.} = \sum_l \frac{1}{\sqrt{2}} \left( \sqrt{1 - 2S_i^{B_l,z} + 2S_i^{A,z} - 4S_i^{A,z} S_i^{B_l,z}} + \sqrt{1 - 2S_i^{A,z} + 2S_i^{B_l,z} - 4S_i^{A,z} S_i^{B_l,z}} \right), \quad (71)$$

similarly,

$$(U_i^{(d)\dagger} U_{i+1}^{(b)})_{\uparrow\downarrow} + \text{H.c.} = \sum_l \frac{1}{\sqrt{2}} \left( \sqrt{1 - 2S_i^{B_l,z} + 2S_{i+1}^{A,z} - 4S_{i+1}^{A,z} S_i^{B_l,z}} + \sqrt{1 - 2S_{i+1}^{A,z} + 2S_i^{B_l,z} - 4S_{i+1}^{A,z} S_i^{B_l,z}} \right). \quad (72)$$

In the presence of an external vector potential  $\mathbf{A}$ , the hopping parameter is modified by the so-called Peierls substitution<sup>61</sup>,  $t \rightarrow t \exp(-i \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A} \cdot d\mathbf{r})$ , where  $\int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A} \cdot d\mathbf{r}$  is the integral of the vector potential along the hopping path, and take account of the possibility of tunneling between neighboring sites. Thus, placing Eqs. (71) and (72) into (70) and making the above substitution, we obtain the following effective  $t$ - $J$  Hamiltonian:

$$\begin{aligned} \mathcal{H}_{eff}^{t-J} = & \frac{-\sqrt{2}te^{-i \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A} \cdot d\mathbf{r}}}{\pi} \sin(\frac{k_F}{2}) \sum_{i;i'=i,i+1;l} \left[ \sqrt{1 - 2S_i^{B_l,z} + 2S_{i'}^{A,z} - 4S_{i'}^{A,z} S_i^{B_l,z}} + \sqrt{1 - 2S_{i'}^{A,z} + 2S_i^{B_l,z} - 4S_{i'}^{A,z} S_i^{B_l,z}} \right] \\ & - J(1-\delta) \sum_i [(\mathbf{S}_{iB_1} + \mathbf{S}_{iB_2}) \cdot (\mathbf{S}_{iA} + \mathbf{S}_{i+1A})] - h_A \sum_i S_i^{A,z} - \sum_{i,l} h_{B_l} S_i^{B_l,z} - J(1-\delta)N_c, \end{aligned} \quad (73)$$

where we have introduced the magnetic field  $h_A$ ,  $h_{B_1}$  and  $h_{B_2}$  for convenience in the calculation of the magnetization. For a given magnetic field, we have the freedom to choose the gauge for  $\mathbf{A}$  that fits best to our needs. A convenient gauge for representing a homogeneous field in the  $z$  direction is the Landau gauge:  $\mathbf{A} = h x \hat{\mathbf{y}}$ , where  $h = -h_A + h_{B_1} + h_{B_2}$ , and the flux per unit cell is  $\phi = ha^2(a \equiv 1)$ . Now, by applying the second-order spin-wave analysis, with the help of Eqs. (38), (39) and (48), we arrive at the following diagonalized Hamiltonian  $\mathcal{H}^t$ :

$$\mathcal{H}^t = -\frac{4\sqrt{2}}{\pi} te^{-(h_A + h_{B_1} + h_{B_2})} \sin(\frac{k_F}{2}) \sum_k \{ 4S - 3v_k^2 - [u_k^2 + 2v_k^2] \alpha_k^\dagger \alpha_k - [2u_k^2 + v_k^2] \beta_k^\dagger \beta_k - \xi_k^\dagger \xi_k \}, \quad (74)$$

and the exchange one,  $\mathcal{H}_2^J$ , becomes:

$$\begin{aligned} \mathcal{H}^J = & (1-\delta) \sum_k \left\{ -J(4S^2 + 1) + JS(\sqrt{9 - 2\gamma_k^2} - 3) + \epsilon_k^{(\alpha)} \alpha_k^\dagger \alpha_k + \epsilon_k^{(\beta)} \beta_k^\dagger \beta_k + \epsilon_k^{(\xi)} \xi_k^\dagger \xi_k \right\} - SN_c [-h_A + h_{B_1} + h_{B_2}] \\ & - h_A \sum_k \left[ v_k^2 \alpha_k^\dagger \alpha_k + v_k^2 + u_k^2 \beta_k^\dagger \beta_k \right] + \frac{1}{2} \sum_{k,l=1,2} h_{B_l} \left[ u_k^2 \alpha_k^\dagger \alpha_k + v_k^2 + v_k^2 \beta_k^\dagger \beta_k + \xi_k^\dagger \xi_k \right] \\ & - \frac{2}{N_c} J(1-\delta) \left[ \left( \sum_k v_k^2 \right)^2 + \left( \sum_k \gamma_k u_k v_k \right)^2 - \frac{3}{\sqrt{2}} \sum_k (v_k^2) \sum_p (\gamma_p u_p v_p) \right]. \end{aligned} \quad (75)$$

Therefore, the energy spectrum of  $\mathcal{H}^t$  in the presence of a magnetic field takes the form:

$$E_1 = -\frac{4\sqrt{2}}{\pi} t e^{-(h_A + h_{B_1} + h_{B_2})} \sin\left(\frac{k_F}{2}\right) \sum_k (4S - 3v_k^2), \quad (76)$$

whereas the one of  $\mathcal{H}^J$  reads:

$$\begin{aligned} E_2 = & -J(4S^2 + 1)(1-\delta)N_c + JS(1-\delta) \sum_k \left[ \sqrt{9 - 8\gamma_k^2} - 3 \right] - SN_c(-h_A + h_{B_1} + h_{B_2}) \\ & + \sum_k v_k^2(-h_A + \frac{1}{2}h_{B_1} + \frac{1}{2}h_{B_2}) - \frac{2}{N_c} J(1-\delta) \left[ \left( \sum_k v_k^2 \right)^2 + \left( \sum_k \gamma_k u_k v_k \right)^2 - \frac{3}{\sqrt{2}} \sum_k (v_k^2) \sum_p (\gamma_p u_p v_p) \right]. \end{aligned} \quad (77)$$

Then, by adding Eqs. (76) and (77), using Eq. (57) and taking the thermodynamic limit, we find the GS energy per unit cell in the presence of a magnetic field:

$$\begin{aligned} E_h/N_c = & -4JS^2(1-\delta) - J(1-\delta) + JS(1-\delta) \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \left( \sqrt{9 - 8\gamma_k^2} - 3 \right) - 2J(1-\delta) \left( q_1^2 + q_2^2 - \frac{3}{\sqrt{2}} q_1 q_2 \right) \\ & - \frac{4\sqrt{2}}{\pi} t e^{-(h_A + h_{B_1} + h_{B_2})} \sin(\pi\delta) (4S - 3q_1) - S(-h_A + h_{B_1} + h_{B_2}) + q_1 \left[ -h_A + \frac{1}{2}h_{B_1} + \frac{1}{2}h_{B_2} \right]. \end{aligned} \quad (78)$$

### A. Doped regime: Ground state energy

Up to this point, we have focused on the development of an analytical approach to investigate the doped  $AB_2$   $t$ - $J$  chain. A *bona fide* analytical model, that takes charge and spin quantum fluctuations into account, must present results that are compatible with numerical and/or experimental studies. For the case at hand, in order to verify the validity of our analytical model, we compare our results with those obtained through numerical techniques using density matrix renormalization group (DMRG) and Lanczos exact diagonalization (ED)<sup>26</sup> of finite systems.

Now, by performing the integration over the first BZ zone in Eq. (78) and setting  $S = 1/2$ , we find that the  $AB_2$   $t$ - $J$  ground state energy per unit cell as a function of hole doping and in zero-field reads:

$$\frac{E_0(\delta)}{JN_c} = -1.9543 \frac{t}{J} \sin(\pi\delta) - 2.4608(1-\delta). \quad (79)$$

We shall now examine the case of small hole doping away from half filling, i.e., with the hole concentration ranging from  $\delta = 0$  up to  $\delta = 0.2$ , for two values of the ratio  $J/t$ : 0.1 and 0.3. Without loss of generality, we set  $t = 1$  in our numerical computations.

In Fig. 1, we show the evolution of the GS energy per unit cell of the  $AB_2$   $t$ - $J$  model as a function of hole doping for the both mentioned values of  $J/t$  in comparison with the numerical results<sup>26</sup>. From the two results at  $J/t = 0.3$ , one can see clearly that the only quantitative difference induced by the increase of the hole concentration is a crossing feature around  $\delta \approx 0.1$ , where our analytical results slightly change its behavior by lowering the energy with respect to the numerical data<sup>26</sup>. Because our model assumes a ferrimagnetic state as starting point, this change of behavior suggests that we have entered in a region of strong magnetic instabilities, and possibly indicating a smooth transition to an incommensurate phase with zero GS total spin beyond  $\delta \approx 0.1$  as confirmed by the numerical data in Ref. (26). On the other hand, at  $J/t = 0.1$ , although our results reproduce the numerical data with some acceptable agreement, we observe a discrepancy that increases with  $\delta$ . The cause of such discrepancy will be discussed in the next subsection.

With the purpose of determining the interplay between the contribution of magnetic exchange and the itinerant kinetic energy, Eqs. (76) and (77), respectively, to the zero-field GS energy Eq. (78), we take  $J/t = 0.3$  and show its evolution with doping in Fig. 2. We can see in the insets, Figs. 2(a) and 2(b), the competitive behavior of

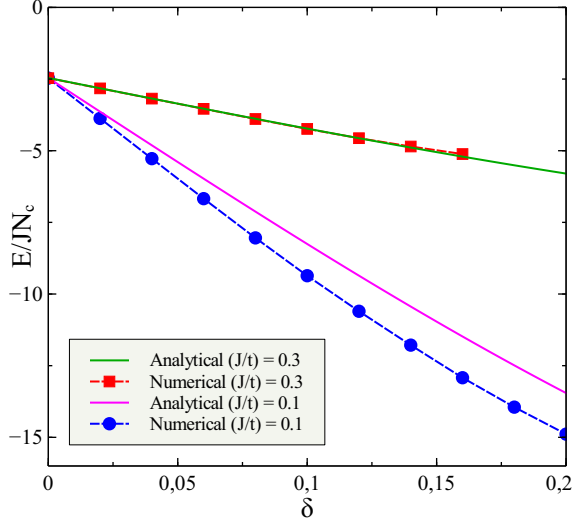


FIG. 1. (Color online) Analytical predictions for the GS energy per unit cell of the doped  $AB_2$   $t$ - $J$  chains as a function of doping, and comparison with numerical data from DMRG and Lanczos techniques for  $J/t = 0.1$  and  $J/t = 0.3$ <sup>26</sup>. In particular, at half filling ( $\delta = 0$ ) the above result agrees very well with the numerical result<sup>26</sup>:  $\approx -2.4678$ . Note that we have added the term  $-JN_c$  with the intention of comparison with numerical calculation.

the two energetic contributions, i.e., the contribution of the exchange energy increases with  $\delta$ , while a practically linear decrease of the hopping term is observed as one enhances the hole doping. This competition indicates that a phase transition to a paramagnetic phase should occur at some critical concentration value.

### B. Doped regime: Ground state total spin

The existence of a transition from modulated itinerant ferrimagnetic phase to an incommensurate paramagnetic phase is a most interesting feature observed numerically in doped  $AB_2$   $t$ - $J$  Hubbard chains<sup>26</sup>. In order to firmly corroborate the mentioned transition, we have calculated the GS total spin per unit cell,  $S_{GS} = \langle S^{A,z} \rangle + \langle S^{B_1,z} \rangle + \langle S^{B_2,z} \rangle$ , by means of the zero-field derivative of Eq. (78):  $\langle S^{A,z} \rangle = -\frac{1}{N_c} \frac{\partial E_h}{\partial h_A} \big|_{h=0}$  and  $\langle S^{B_{1,2},z} \rangle = -\frac{1}{N_c} \frac{\partial E_h}{\partial h_{B_{1,2}}} \big|_{h=0}$ . Indeed, we find

$$\frac{S_{GS}(\delta)}{S_L} = 1 - 3.9086 \sin(\pi\delta). \quad (80)$$

In Fig. 3 we plot the evolution of  $S_{GS}$ , normalized by its value in the undoped regime (Lieb GS total spin  $S_L = \frac{1}{2}$ ), as a function of  $\delta$ , and compare it with the numerical data from DMRG and Lanczos techniques<sup>26</sup>, for  $J/t = 0.3$  (red squares) and  $J/t = 0.1$  (blue circles). In the latter (former) case, the system undergoes

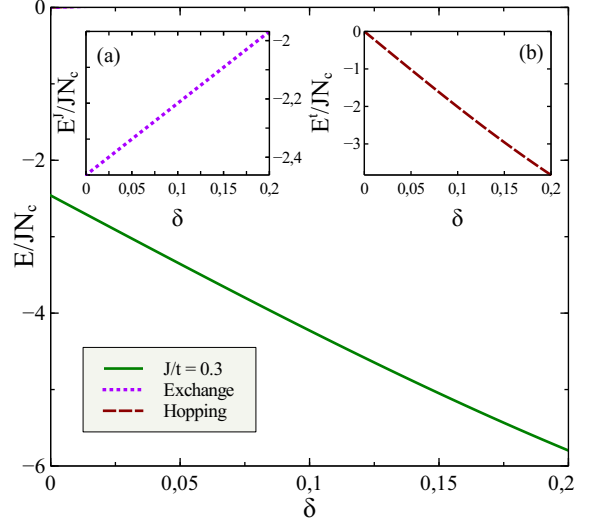


FIG. 2. (Color online) Ground-state energy per unit cell for the  $AB_2$   $t$ - $J$  chains as a function of  $\delta$  for  $J/t = 0.3$ . In the insets, we illustrate the two energetic contribution due to (a) exchange and (b) hopping terms.

a transition from the itinerant ferrimagnetic phase to an incommensurate phase with zero (nonzero)  $S_{GS}$ .

We can observe that, as one increases the hole doping, the value of  $S_{GS}$  decreases linearly until the magnetic order is completely suppressed at  $\delta_c \approx 0.08$ . This behavior is supported by the numerical results<sup>26</sup>, particularly in the regime where the Nagaoka phenomenon is not manifested, that is, at  $J/t = 0.3$ . In this regime, spin and charge quantum fluctuations destabilize the ferrimagnetic structure and triggers a transition to an incommensurate paramagnetic phase at  $\delta_c$ , with  $S_{GS} \sim (\delta - \delta_c) \rightarrow 0$ . Moreover, we stress that, charge and spin quantum fluctuations are practically decoupled, as indicated by the formation of hole (charge) density wave in anti-phase with the modulation of the ferrimagnetic structure<sup>26</sup>. At  $J/t = 0.1$  and  $\delta > 0.1$ , however, the formation of magnetic polarons (onset of the Nagaoka phenomena that sets in as  $U \rightarrow \infty$ ) with charge-density waves in phase with the modulation of the ferrimagnetic structure, as indicated by the DMRG data<sup>26</sup>, that leads to an incommensurate phase with nonzero  $S_{GS}$ .

## VI. CONCLUSIONS

In summary, we have presented a detailed analytical study of the large- $U$  Hubbard model on the quasi-one-dimensional  $AB_2$  chain. We used a functional integral approach combined with a perturbative expansion in the strong-coupling regime that allowed us to properly analyze the referred system at and away from half filling.

At half filling, our model is mapped onto the quantum Heisenberg model, suitable analyzed through a spin-wave

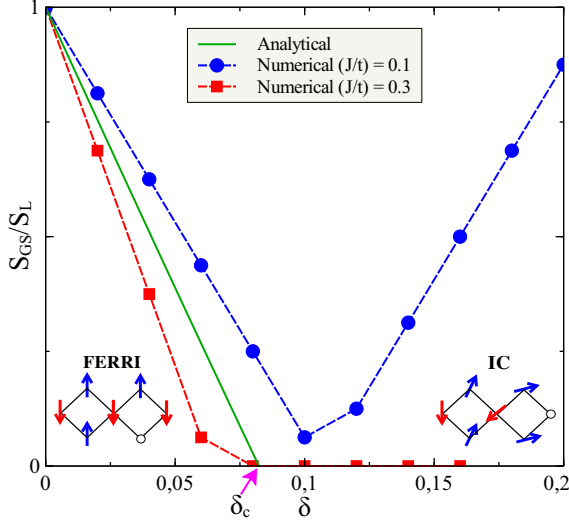


FIG. 3. (Color online) Ground-state total spin  $S_{GS}$  per unit cell (solid green line), normalized by its value in the undoped regime:  $S_L = \frac{1}{2}$ , as a function of hole doping  $\delta$  for the indicated values of  $J/t$ .

perturbative series expansion in powers of  $1/S$ . We find that the GS energy and sublattice magnetizations are in very good agreement with previous results. In addition, our analytical results for the GS energy and total spin per unit cell as a function of hole doping are in very good agreement with recent numerical calculations, particularly in the regime where the Nagaoka phenomenon is not manifested. In fact, in this challenging regime we have demonstrate that our approach treats the interplay between charge and spin quantum fluctuations on equal footing, and that these fluctuations effectively drives the breakdown of the ferrimagnetic order at a critical hole concentration, thus signaling a smooth transition to a paramagnetic phase. We also remark that, in the doped regime charge and spin quantum fluctuations are practically decoupled, as numerically indicated by the formation of hole (charge) density waves in anti-phase with the modulation of the ferrimagnetic structure.

Finally, we would like to stress that the reported results strongly suggest that the approach used in a very recent study on the compatibility between numerical and analytical outcomes of the large- $U$  Hubbard model on the honeycomb lattice (a two-dimensional system at half filling and in the hole-doped regime), was proved suitable for the  $AB_2$  chain (a quasi-one-dimensional system), where the impact of charge and spin quantum fluctuations are expected to manifest in a stronger way.

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#### Appendix: Perturbative expansion of $\mathcal{L}_n(\tau)$

In this appendix we present the main steps of the derivation of the perturbative expansion of  $\mathcal{L}_n$ , in Eq. (11), up to  $\mathcal{O}(J)$ . In direct connection with the transformations in Eq. (13), it is convenient to define rotation matrices either symmetric or antisymmetric with respect to the exchange operation  $B_1 \leftrightarrow B_2$ :

$$U_i^{(b)} = U_{iA},$$

$$U_i^{(d,e)} = \frac{1}{\sqrt{2}}(U_{iB_1} \pm U_{iB_2}). \quad (\text{A.1})$$

In the sequence, by substituting both the above transformations and its analogous in Eq. (13) into Eq. (11), we find that  $\mathcal{L}_n(\tau)$  can be written as the sum of the following nine terms

$$\mathcal{L}_n(\tau) = \mathcal{L}_n^{(1)} + \mathcal{L}_n^{(2)} + \mathcal{L}_n^{(3)} + \mathcal{L}_n^{(4)} + \mathcal{L}_n^{(5)} + \mathcal{L}_n^{(6)} + \mathcal{L}_n^{(7)} + \mathcal{L}_n^{(8)} + \mathcal{L}_n^{(9)}, \quad (\text{A.2})$$

where

$$\begin{aligned} \mathcal{L}_n^{(1)} &= \sum_{i\sigma\sigma'} b_{i\sigma'}^\dagger (U_i^{(b)\dagger} \partial_\tau U_i^{(b)})_{\sigma'\sigma} b_{i\sigma}, \\ \mathcal{L}_n^{(2)} &= \frac{1}{2} \sum_{i\sigma\sigma'} d_{i\sigma'}^\dagger [U_i^{(d)\dagger} \partial_\tau U_i^{(d)} + U_i^{(e)\dagger} \partial_\tau U_i^{(e)}] d_{i\sigma}, \\ \mathcal{L}_n^{(3)} &= \frac{1}{2} \sum_{i\sigma\sigma'} e_{i\sigma'}^\dagger [U_i^{(d)\dagger} \partial_\tau U_i^{(d)} + U_i^{(e)\dagger} \partial_\tau U_i^{(e)}] e_{i\sigma}, \\ \mathcal{L}_n^{(4)} &= \frac{1}{2} \sum_{i\sigma\sigma'} d_{i\sigma'}^\dagger [U_i^{(d)\dagger} \partial_\tau U_i^{(e)} + U_i^{(e)\dagger} \partial_\tau U_i^{(d)}] e_{i\sigma}, \\ \mathcal{L}_n^{(5)} &= \frac{1}{2} \sum_{i\sigma\sigma'} e_{i\sigma'}^\dagger [U_i^{(d)\dagger} \partial_\tau U_i^{(e)} + U_i^{(e)\dagger} \partial_\tau U_i^{(d)}] d_{i\sigma}, \\ \mathcal{L}_n^{(6)} &= -t \sum_{i\sigma\sigma'} [b_{i\sigma'}^\dagger (U_i^{(b)\dagger} U_i^{(d)} - \sqrt{2})_{\sigma'\sigma} d_{i\sigma} + \text{H.c.}], \\ \mathcal{L}_n^{(7)} &= -t \sum_{i\sigma\sigma'} [b_{i\sigma'}^\dagger (U_i^{(b)\dagger} U_i^{(e)})_{\sigma'\sigma} e_{i\sigma} + \text{H.c.}], \\ \mathcal{L}_n^{(8)} &= -t \sum_{i\sigma\sigma'} [d_{i\sigma'}^\dagger (U_i^{(d)\dagger} U_{i+1}^{(b)} - \sqrt{2})_{\sigma'\sigma} b_{i+1\sigma} + \text{H.c.}], \\ \mathcal{L}_n^{(9)} &= -t \sum_{i\sigma\sigma'} [e_{i\sigma'}^\dagger (U_i^{(e)\dagger} U_{i+1}^{(b)})_{\sigma'\sigma} b_{i+1\sigma} + \text{H.c.}]. \end{aligned}$$

Now, by inserting the expansions (27) and (28) into the above Lagrangians, and neglecting terms containing exclusively fields related to the high-energy bands,  $\mathcal{L}_n(\tau)$



can be written in terms of the spinless Grassmann fields in a perturbative expansion up to order  $J$  as follows

$$\mathcal{L}_n^{(1)} = \sum_{i\sigma} \theta(-\sigma) (U_i^{(b)\dagger} \partial_\tau U_i^{(b)})_{\sigma,\sigma} \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^{(\frac{1}{2})}, \quad (\text{A.3})$$

$$\mathcal{L}_n^{(2)} = \sum_{i\sigma;\nu=d,e} \frac{\theta(\sigma)}{2} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma,\sigma} \alpha_i^\dagger \alpha_i, \quad (\text{A.4})$$

$$\mathcal{L}_n^{(3)} = \sum_{i\sigma;\nu=d,e} \frac{\theta(\sigma)}{2} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma,\sigma} e_{i\uparrow}^\dagger e_{i\uparrow}, \quad (\text{A.5})$$

$$\mathcal{L}_n^{(4)} = \sum_{i\sigma;\nu,\nu'=d,e} \frac{\theta(\sigma)}{2} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu')})_{\sigma,\sigma} \alpha_i^\dagger e_{i\uparrow}, \quad (\text{A.6})$$

$$\mathcal{L}_n^{(5)} = [\mathcal{L}_n^{(4)}]^\dagger, \quad (\text{A.7})$$

$$\begin{aligned} \mathcal{L}_n^{(6)} = & - \sum_{i\sigma\sigma'} \left( U_i^{(b)\dagger} U_i^{(d)} - \sqrt{2} \right)_{\sigma,\sigma'} \left\{ t\delta_{\sigma',\sigma} [\theta(-\sigma) \alpha_i^{(\frac{1}{2})\dagger} \beta_i \right. \\ & - \theta(\sigma) \beta_i^{(\frac{1}{2})\dagger} \alpha_i] + t\theta(-\sigma) \delta_{\sigma',-\sigma} \alpha_i^{(\frac{1}{2})\dagger} \alpha_i \\ & + \sqrt{2} \frac{t^2}{U} \delta_{\sigma',\sigma} \left[ \theta(-\sigma) \alpha_i^{(\frac{1}{2})\dagger} (\alpha_i^{(\frac{1}{2})} + \alpha_{i+1}^{(\frac{1}{2})}) \right. \\ & \left. \left. + \theta(\sigma) (\alpha_i^\dagger + \alpha_{i-1}^\dagger) \alpha_i \right] + \text{H.c.} \right\}, \quad (\text{A.8}) \end{aligned}$$

$$\begin{aligned} \mathcal{L}_n^{(7)} = & - \sum_{i\sigma\sigma'} \left( U_i^{(b)\dagger} U_i^{(e)} \right)_{\sigma,\sigma'} \left\{ t\theta(-\sigma) \delta_{\sigma',-\sigma} \alpha_i^{(\frac{1}{2})\dagger} e_{i\uparrow} \right. \\ & + t\delta_{\sigma',\sigma} [\theta(-\sigma) \alpha_i^{(\frac{1}{2})\dagger} e_{i\downarrow} - \theta(\sigma) \beta_i^{(\frac{1}{2})\dagger} e_{i\uparrow}] \\ & \left. + \sqrt{2} \frac{t^2}{U} \delta_{\sigma',\sigma} \theta(\sigma) (\alpha_i^\dagger + \alpha_{i-1}^\dagger) e_{i\uparrow} + \text{H.c.} \right\}, \quad (\text{A.9}) \end{aligned}$$

$$\begin{aligned} \mathcal{L}_n^{(8)} = & - \sum_{i\sigma\sigma'} \left( U_i^{(d)\dagger} U_{i+1}^{(b)} - \sqrt{2} \right)_{\sigma,\sigma'} \left\{ t\delta_{\sigma',\sigma} [\theta(-\sigma) \beta_i^\dagger \alpha_{i+1}^{(\frac{1}{2})} \right. \\ & - \theta(\sigma) \alpha_i^\dagger \beta_{i+1}^{(\frac{1}{2})}] + t\theta(\sigma) \delta_{\sigma',-\sigma} \alpha_i^\dagger \alpha_{i+1}^{(\frac{1}{2})} \\ & + \sqrt{2} \frac{t^2}{U} \delta_{\sigma',\sigma} \left[ \theta(\sigma) \alpha_i^\dagger (\alpha_i + \alpha_{i+1}) \right. \\ & \left. + \theta(-\sigma) (\alpha_i^{(\frac{1}{2})\dagger} + \alpha_{i+1}^{(\frac{1}{2})\dagger}) \alpha_{i+1}^{(\frac{1}{2})} \right] + \text{H.c.} \right\}, \quad (\text{A.10}) \end{aligned}$$

$$\begin{aligned} \mathcal{L}_n^{(9)} = & - \sum_{i\sigma\sigma'} \left( U_i^{(e)\dagger} U_{i+1}^{(b)} \right)_{\sigma,\sigma'} \left\{ t\theta(\sigma) \delta_{\sigma',-\sigma} e_{i\uparrow}^\dagger \alpha_{i+1}^{(\frac{1}{2})} \right. \\ & + t\delta_{\sigma',\sigma} [\theta(-\sigma) e_{i\downarrow}^\dagger \alpha_{i+1}^{(\frac{1}{2})} - \theta(\sigma) e_{i\uparrow}^\dagger \beta_{i+1}^{(\frac{1}{2})}] \\ & \left. + \sqrt{2} \frac{t^2}{U} \delta_{\sigma',\sigma} \theta(\sigma) e_{i\uparrow}^\dagger (\alpha_i + \alpha_{i+1}) + \text{H.c.} \right\} \quad (\text{A.11}) \end{aligned}$$

We remark that, in Eqs. (A.3)-(A.7) multiplicative terms of  $\mathcal{O}(t/U)$  were neglected, since  $(U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma,\sigma}$  scale with  $J$  [see Eq. (33)]. However, as we can see in the above equations, terms allowing interband transitions between low- and high-energy bands do exist in  $\mathcal{L}_n$ . In the following, we present the perturbative scheme<sup>42-44</sup> suitable to eliminate the referred high-energy states.

We consider that in the unperturbed ferrimagnetic state  $|\Phi_0(N)\rangle$  at half-filled band ( $N_e = N$  electrons) and total energy  $E_0(N)$ , the low-energy electronic modes  $(\alpha_k, e_{k\uparrow})$  are filled, while the high-energy  $(\beta_k, e_{k\downarrow})$  ones are empty. In the context of a second-order Rayleigh-Schrödinger perturbation theory, consistent with the strong-coupling expansion up to  $\mathcal{O}(t^2/U)$ , the virtual excited states  $|\gamma_k, \sigma\rangle$  contain  $N-1$  electrons in the low-energy bands and one electron with spin  $\sigma$  promoted to a high-energy band: either  $\beta$  [with energy  $E_k^\gamma = E_0(N-1) + E_k + U/2$ ] or  $e_{k\downarrow}$  [with  $E_k^\gamma = E_0(N-1) + U$ ]. Contributions to the perturbative Hamiltonian  $H_1$  (see below) are thus generated from terms in Eqs. (A.8)-(A.11). Therefore, the energy shift or effective Hamiltonian, derived through  $\Delta E = \sum_{k\sigma} \frac{\langle \Phi_0 | H_1 | \gamma_k, \sigma \rangle \langle \gamma_k, \sigma | H_1 | \Phi_0 \rangle}{E_0 - E_k^\gamma} \rightarrow \mathcal{H}_{eff}$ , is identical to Eq. (32d), after cancellation of extra contributions from  $\Delta E$  and the last terms of Eqs. (A.8)-(A.11), so that the remained terms in Eq. (32d) give rise to the exchange quantum Heisenberg model at half filling in Sec. (IV).

Under the above scheme, the perturbative expansion of  $\mathcal{L}_n(\tau)$  obtains in terms of lower-energy bands only, whose sum with  $\mathcal{L}_0(\tau)$ , Eq. (30), results in  $\mathcal{L}_{eff}(\tau)$ , Eq. (31).

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